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MEMORANDUM
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THE THERMODYNAMICS OF
THE POLYSTYRENE-HYDROCARBON
VAPOR SYSTEM

F. J. Krieger

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PREFACE

This study was done at the request of the Scientific Advisor to the Physics Division, Research Directorate, Air Force Special Weapons Center, Kirtland Air Force Base, New Mexico.

It is a contribution to a better understanding of the complex problems involved in the physics of re-entry bodies. Polystyrene is the second of a series of ablative materials to be investigated by means of mathematical techniques similar to those used at RAND in the parametric study of certain low-molecular-weight compounds as nuclear rocket propellants.

The results of investigations of graphite and polyethylene are reported in RAND Memorandums RM-3326-PR, The Thermodynamics of the Graphite-Carbon Vapor System, and RM-3709-PR, The Thermodynamics of the Polyethylene-Hydrocarbon Vapor System.

SUMMARY

The purpose of this study is the thermodynamic investigation of polystyrene over a range of temperatures up to 6000°K and pressures up to 10^6 atmospheres.

Two sets of equilibrium composition equations are used--one representing a pure gas phase, the other a heterogeneous system of gas and solid carbon. The gas phase of the heterogeneous chemical system, like the homogeneous gas phase, comprises 70 gaseous carbon and hydrocarbon species.

The results of the computational program are presented in both tabular and graphic form. The latter is a conventional Mollier diagram in which specific enthalpy is plotted against specific entropy, with cross plots of temperature, pressure, and molecular weight.

ACKNOWLEDGMENTS

This study involved considerable hand and machine computation. The efforts of the following RAND Physics Department staff members are gratefully acknowledged: Donald A. Brown, for his extensive liaison and computational work; and Elizabeth J. Force, for her meticulous graphical presentation of the tabulated results.

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I. INTRODUCTION

This study considers a chemical system that under certain conditions of temperature and pressure is a pure gas mixture and under others is a disperse system, or smoke. In this case the smoke is a gas that contains a condensed phase, solid carbon or graphite, symbolized by C_s .

In deriving the computations, the following assumptions have been made:

- (1) Thermal equilibrium is maintained between the solid particles and the gas phase.
- (2) The pressure due to the thermal motion of the solid particles can be neglected.
- (3) The gas phase obeys the ideal-gas law.
- (4) The molar volume of solid carbon is essentially constant, that is, independent of temperature and pressure.

II. COMPOSITION EQUATIONS

In this study it is assumed that the gas formed by heating polystyrene, whose molecular formula is $[C_8H_8]_x$ or, simply, CH , at various pressures up to a temperature of $6000^\circ K$ is a mixture of H , H_2 , C_s (graphite), C (gas), and 67 other carbon and hydrocarbon chemical species for which thermochemical data are available. The presence or absence of a condensed phase makes it necessary to consider two distinct sets of chemical equations.

A. Solid carbon present. In terms of H_2 and C_s as independent components, the chemical equations for the dependent, or derived, components are given by the expression

$$a_i C_s + b_i H_2 = C_{a_i} H_{2b_i}, \quad (1)$$

where a_i has the integral values 0, 1, 2, ..., and b_i has the half-integral values 0, 1/2, 1, 3/2,

The equations required to determine the equilibrium composition of the nonhomogeneous gas mixture are obtained from mass-balance and equilibrium considerations. The following two equations are derived from mass-balance considerations:

$$n_s = 1 - \sum_{i=1}^{69} a_i n_i, \quad (2)$$

and

$$n_{H_2} = 1/2 - \sum_{i=1}^{69} b_i n_i, \quad (3)$$

where n_s is the number of moles of C_s , a_i is the coefficient of C_s on the left-hand side of Eq. (1), n_{H_2} is the number of moles of H_2 , b_i is the coefficient of H_2 on the left-hand side of Eq. (1), and n_i is the corresponding number of moles of component i .

The equilibrium equations are obtained by considering the free energy F of the system and the partial molar free energy of chemical potential $\mu_j = \partial F / \partial n_j$ of each component. The chemical potential is a

function of the state and composition of the system. For an ideal gas

$$\mu_i = \mu_i^0 + RT \ln (n_i P/n), \quad i = H_2, 1, \dots, 69, \quad (4)$$

where μ_i^0 is the chemical potential of component i in the standard state of unit partial pressure, R is the gas constant, T is the temperature, P is the pressure, and n is the total number of moles of gas in the mixture.

The chemical potential for graphite is given by

$$\mu_s = \mu_s^0 + (P - 1)\bar{v}_s, \quad (5)$$

where μ_s^0 is the standard molar free energy for graphite, \bar{v}_s is the molar volume of graphite, and P is the pressure of the system.

The condition for chemical equilibrium is that for all possible reactions represented by Eq. (1),

$$\Delta F = \sum \mu_j \Delta n_j = 0, \quad j = C_s, H_2, 1, \dots, 69, \quad (6)$$

at constant temperature and pressure. Equations (4) and (5) may, therefore, be combined to give

$$\begin{aligned} RT \ln (n_i P/n) = a_1 \mu_s^0 + b_1 \mu_{H_2}^0 - \mu_i^0 + a_1 (P - 1)\bar{v}_s \\ + b_1 RT \ln (n_{H_2} P/n). \end{aligned} \quad (7)$$

Because the equilibrium constants K_1 associated with the chemical reactions (1) are defined by the relation

$$\Delta F^0 = \mu_i^0 - a_1 \mu_s^0 - b_1 \mu_{H_2}^0 = - RT \ln K_1, \quad (8)$$

Eq. (7) may be written in the form

$$\ln (n_i P/n) = \ln K_i + a_i (P - 1) \bar{V}_s / RT + b_i \ln (n_{H_2} P/n), \quad (9)$$

or

$$n_i = K_i \exp \left[a_i (P - 1) \bar{V}_s / RT \right] (P/n)^{b_i - 1} (n_{H_2})^{b_i}. \quad (10)$$

Equations (2), (3), and (10) form a system of 71 non-linear equations in 71 unknowns which can be solved by a process of iteration.

B. Solid carbon absent. In terms of H_2 and C (gas) as independent components, the chemical equations for the dependent, or derived, components are given by the expression

$$a_j C + b_j H_2 = C_{a_j} H_{2b_j}, \quad (11)$$

where a_j has the integral values 0, 1, 2, ..., and b_j has the half-integral values 0, 1/2, 1, 3/2,

The mass-balance equations are

$$n_C = 1 - \sum a_j n_j, \quad (12)$$

and

$$n_{H_2} = 1/2 - \sum b_j n_j, \quad (13)$$

where n_C is the number of moles of C, a_j is the coefficient of C on the left-hand side of Eq. (11), n_{H_2} is the number of moles of H_2 , b_j is the coefficient of H_2 on the left-hand side of Eq. (11), and n_j is the corresponding number of moles of component 'j'.

The equilibrium equations are given by the expression

$$n_j = K_j (P/n)^{a_j + b_j - 1} (n_C)^{a_j} (n_{H_2})^{b_j}, \quad (14)$$

where n is the total number of moles of gas in the equilibrium

mixture, P is the total pressure in atmospheres, and K_j is the thermodynamic equilibrium constant of component j . These values of K_j are quite different from those in Eq. (10) because of the reactions with which they are associated.

III. THERMODYNAMIC EQUATIONS

The molecular weight of the gas mixture is given by the relation

$$M = \frac{13.019}{\bar{n}}, \quad (15)$$

where 13.019 is the formula weight of the input material CH and \bar{n} is the total number of moles in the gas mixture, including C_s .

The specific free energy (in calories per gram) of the gas mixture is given by the expression

$$f = \frac{1}{13.019} \left\{ \sum_i^g n_i [\mu_i^0 + RT \ln (n_i P/n)] + n_s [\mu_s^0 + c(P - 1)\bar{v}_s] \right\}, \quad (16)$$

which is derived from Eqs. (4) and (5). The summation is over all gaseous species. The constant $c = 0.0242172$ converts cc-atmospheres to calories.

The specific entropy (in calories per degree per gram) of the gas mixture is given by the expression

$$s = \frac{1}{13.019} \left\{ \sum_i^g n_i [S_i^0 - R \ln (n_i P/n)] + n_s [S_s^0 - \alpha_v(P - 1)\bar{v}_s] \right\}, \quad (17)$$

where S_i^0 and S_s^0 are the standard molar entropy of component i and graphite, respectively, at a given temperature, and α_v is the volume coefficient of thermal expansion of graphite.

The specific enthalpy (in calories per gram) of the gas mixture is given by the expression

$$h = \frac{1}{13.019} \left\{ \sum_i^g n_i H_i^0 + n_s [H_s^0 + c(1 - \alpha_v T)(P - 1)\bar{v}_s] \right\}, \quad (18)$$

where H_i^0 and H_s^0 are the standard molar heat content of component i and graphite, respectively, at a given temperature.

The specific internal energy (in calories per gram) of the gas mixture is given by the expression

$$u = \frac{1}{13.019} \left\{ \sum^g n_i (H_i^O - RT) + n_s [H_s^O - c[1 + (P - 1)\alpha_v T]\bar{V}_s] \right\}. \quad (19)$$

The terms representing the increase in a thermodynamic property from one atmosphere to P atmospheres for graphite, namely,

$$\Delta F = (P - 1)\bar{V}_s, \quad (20)$$

$$\Delta S = -\alpha_v(P - 1)\bar{V}_s, \quad (21)$$

$$\Delta H = (1 - \alpha_v T)(P - 1)\bar{V}_s, \quad (22)$$

$$\Delta U = -\alpha_v T(P - 1)\bar{V}_s, \quad (23)$$

are readily derived from the differential formulas relating the various thermodynamic functions. Each of the above terms must be multiplied by the factor $c = 0.0242172$ to convert it from cc-atmospheres to calories.

The specific volume of the gas mixture (in cubic centimeters per gram) is given by the expression

$$v = \frac{1}{13.019} \left\{ nRT/P + n_s \bar{V}_s \right\}, \quad (24)$$

where the first term in the brackets is the volume of the gas phase and the second term is that of the solid phase.

IV. BASIC DATA

The pertinent thermodynamic properties (heat content, entropy, free energy, and heat of formation) for the 71 chemical species considered in this study were taken partly from JANAF Thermochemical Data⁽¹⁾ and partly from Los Alamos Scientific Laboratory Report LA-2556.⁽²⁾ In the latter report the thermodynamic functions are expressed in polynomial form. The molecular weights and heats of formation of the various components are listed in the following table. The isomeric forms of certain species are listed in the same order as they appear in Tables III and IV of the LASL report.

	<u>Component</u>	<u>Molecular Weight</u>	<u>Heat of Formation at 0°K (cal/mole)</u>	<u>Reference</u>
1.	H	1.008	51,632	1
2.	H ₂	2.016	0	1
3.	C _s (graphite)	12.011	0	1
4.	C	12.011	169,576	1
5.	CH	13.019	141,183	1
6.	CH ₂	14.027	67,015	1
7.	CH ₃	15.035	32,805	1
8.	CH ₄	16.043	-15,991	1
9.	C ₂	24.022	197,000	1
10.	C ₂ H	25.030	116,700	2
11.	C ₂ H ₂	26.038	54,325	1
12.	C ₂ H ₃	27.046	66,900	2
13.	C ₂ H ₄	28.054	14,520	1
14.	C ₂ H ₆	30.070	-16,517	2
15.	C ₃	36.033	188,104	1
16.	C ₃ H	37.041	127,100	2
17.	C ₃ H ₂	38.049	106,700	2
18.	C ₃ H ₃	39.057	77,300	2
19.	C ₃ H ₄	40.065	46,017	2
20.	C ₃ H ₄	40.065	47,700	2
21.	C ₃ H ₅	41.073	34,900	2
22.	C ₃ H ₆	42.081	8,468	2

	Component	Molecular Weight	Heat of Formation at 0°K (cal/mole)	Reference
23.	C ₃ H ₆	42.081	17,800	2
24.	C ₃ H ₈	44.097	-19,482	2
25.	C ₄	48.044	240,500	1
26.	C ₄ H	49.052	154,000	2
27.	C ₄ H ₂	50.060	111,300	2
28.	C ₄ H ₃	51.068	102,500	2
29.	C ₄ H ₄	52.076	75,300	2
30.	C ₄ H ₄	52.076	71,300	2
31.	C ₄ H ₅	53.084	67,800	2
32.	C ₄ H ₅	53.084	67,400	2
33.	C ₄ H ₆	54.092	38,090	2
34.	C ₄ H ₆	54.092	42,740	2
35.	C ₄ H ₆	54.092	29,780	2
36.	C ₄ H ₆	54.092	42,000	2
37.	C ₄ H ₈	56.108	3,480	2
38.	C ₄ H ₈	56.108	4,960	2
39.	C ₄ H ₈	56.108	980	2
40.	C ₄ H ₈	56.108	2,240	2
41.	C ₄ H ₈	56.108	12,500	2
42.	C ₄ H ₁₀	58.124	-23,670	2
43.	C ₄ H ₁₀	58.124	-25,300	2
44.	C ₅	60.055	240,298	1
45.	C ₅ H	61.063	185,400	2
46.	C ₅ H ₂	62.071	165,000	2
47.	C ₅ H ₃	63.079	135,600	2
48.	C ₅ H ₄	64.087	103,600	2
49.	C ₅ H ₄	64.087	108,300	2
50.	C ₅ H ₄	64.087	102,300	2
51.	C ₅ H ₆	66.103	25,200	2
52.	C ₆	72.066	287,000	2
53.	C ₆ H	73.074	211,300	2
54.	C ₆ H ₂	74.082	168,600	2
55.	C ₆ H ₃	75.090	158,300	2

	Component	Molecular Weight	Heat of Formation at 0°K (cal/mole)	Reference
56.	C ₆ H ₄	76.098	132,000	2
57.	C ₆ H ₄	76.098	132,800	2
58.	C ₆ H ₄	76.098	124,000	2
59.	C ₆ H ₆	78.114	24,000	2
60.	C ₇	84.077	287,000	2
61.	C ₇ H	85.085	240,000	2
62.	C ₇ H ₂	86.093	220,000	2
63.	C ₈	96.088	339,000	2
64.	C ₈ H	97.096	267,000	2
65.	C ₈ H ₂	98.104	225,000	2
66.	C ₉	108.099	334,000	2
67.	C ₉ H	109.107	291,000	2
68.	C ₉ H ₂	110.115	271,000	2
69.	C ₁₀	120.110	393,000	2
70.	C ₁₀ H	121.118	324,000	2
71.	C ₁₀ H ₂	122.126	282,000	2

The molar volume of graphite ($\bar{V}_g = 5.5524$ cc) was derived from a mean density of 2.1632 gm/cc based on measurements of 49 samples at the Los Alamos Scientific Laboratory.⁽³⁾

The volume coefficient of thermal expansion for graphite is given by the expression

$$\alpha_v = \frac{1}{v} \left[\frac{\partial v}{\partial T} \right]_p = (18.80 + 0.001875T) \times 10^{-6} \text{ cc/cc-deg} \quad (25)$$

for $T > 773^\circ\text{K}$. This expression was derived from data on the linear coefficient of expansion of lampblack obtained at the National Carbon Research Laboratories.⁽⁴⁾

Two values of the gas constant were used: $R = 1.98726$ cal/deg-mole and $R = 82.0597$ cc-atm/deg-mole. Their ratio gives the conversion factor $c = 0.0242172$.

V. COMPUTATIONAL PROCEDURE

The two sets of equilibrium composition equations--the one involving solid carbon and the other gaseous species only--represent two mutually exclusive contiguous regions. It is expedient to determine the border line between the two regions, that is, the conditions of temperature and pressure under which solid carbon just vanishes.

This can be done by making use of the fact that under certain conditions the value of n_g in Eq. (2) changes sign. Thus, for a specified pressure, a temperature interval can be found in which the change of sign occurs. If this interval is divided into, say, three equally spaced temperatures, the sublimation temperature of graphite (that is, the temperature at which graphite disappears) at any desired pressure may be determined by interpolation. Thus, at 10^{-3} atm the sublimation temperature is 2990°K , at one atm it is 3524°K , while at 10^3 atm it is 4128°K . It is interesting to note that in the graphite-carbon vapor system⁽⁵⁾ the corresponding temperatures are 3151°K , 4127°K , and 5908°K , respectively.

VI. RESULTS

The results of this study are presented numerically in Tables 1 and 2 and graphically in Figs. 1 and 2. Figure 1 is a conventional Mollier diagram for polystyrene; specific enthalpy is plotted against specific entropy, with cross plots of temperature, pressure, and molecular weight. The temperatures range from 6000°K to 500°K ; the pressures from 10^6 atm to 10^{-8} atm. The dotted line demarcates the pure gas phase (above) from the smoke (below). The cross plots of constant molecular weight represent chemical composition and reflect the increase in concentration of the larger molecules (C_3 through C_{10}) with increase in temperature and pressure, particularly in the vicinity of the gas-smoke borderline. Figure 2 is a plot of volume against temperature with cross plots of constant pressure.

All the computations required to obtain the results in Tables 1 and 2 were made on the RAND JOHNNIAC computer. In the tables the numbers are represented in "floating decimal" notation; the first two digits, minus 50, indicate a power of 10, and the next five digits indicate the decimal form of the number. Thus 5512345 represents 0.12345×10^5 and 4512345 represents 0.12345×10^{-5} .

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Table 1

SUMMARY OF COMPUTED VALUES OF VOLUME, MOLECULAR WEIGHT, MOLES OF GAS,
AND MOLES OF SOLID CARBON FOR POLYSTYRENE AT VARIOUS
TEMPERATURES AND PRESSURES

Tempera- ture, T (°K)	Pressure, P (atm)	Volume, v (cc/gm)	Molecular Weight, M	Moles of Gas, n	Moles of Solid, n _s
546000	56999999	49120740	52407781	50319264	00000000
546000	55999999	50170423	52288903	50450634	00000000
546000	54999999	51221379	52222404	50585373	00000000
546000	53999999	52280161	52175740	50740907	00000000
546000	52999999	53439597	52112002	51116238	00000000
546000	51999999	54680871	51723129	51180036	00000000
546000	50999999	55746210	51659811	51197313	00000000
546000	49999999	56755305	51651866	51199718	00000000
546000	48999999	57756261	51651041	51199971	00000000
546000	47999999	58756358	51650958	51199997	00000000
546000	46999999	59756367	51650950	51199999	00000000
546000	45999999	60756368	51650949	51200000	00000000
546000	44999999	61756368	51650949	51200000	00000000
546000	44100000	62756368	51650949	51200000	00000000
546000	43100000	63756368	51650949	51200000	00000000
545500	56999999	49105883	52426248	50305432	00000000
545500	55999999	50147569	52305841	50425678	00000000
545500	54999999	51192913	52233954	50556476	00000000
545500	53999999	52234031	52192849	50675085	00000000
545500	52999999	53320056	52141015	50923232	00000000
545500	51999999	54541684	51833194	51156254	00000000
545500	50999999	55667816	51675826	51192638	00000000
545500	49999999	56690469	51653654	51199172	00000000
545500	48999999	57693047	51651222	51199916	00000000
545500	47999999	58693308	51650977	51199991	00000000
545500	46999999	59693335	51650952	51199999	00000000
545500	45999999	60693337	51650950	51199999	00000000
545500	44999999	61693337	51650949	51200000	00000000
545500	44100000	62693337	51650949	51200000	00000000
545500	43100000	63693337	51650949	51200000	00000000
545000	56999999	48918770	52446573	50291530	00000000
545000	55999999	50125644	52326555	50398676	00000000
545000	54999999	51166390	52246587	50527967	00000000
545000	53999999	52197471	52207776	50626587	00000000
545000	52999999	53244537	52167785	50775930	00000000
545000	51999999	54370013	52110887	51117407	00000000
545000	50999999	55560793	51731639	51177942	00000000

Table 1--continued

Tempera- ture, T ($^{\circ}$ K)	Pressure, P (atm)	Volume, v (cc/gm)	Molecular Weight, M	Moles of Gas, n	Moles of Solid, n _s
545000	49999999	56620908	51660804	51197017	00000000
545000	48999999	57629327	51651963	51199689	00000000
545000	47999999	58630208	51651051	51199968	00000000
545000	47100000	59630297	51650960	51199996	00000000
545000	46100000	60630306	51650950	51199999	00000000
545000	45100000	61630307	51650949	51200000	00000000
545000	44100000	62630307	51650949	51200000	00000000
545000	43100000	63630307	51650949	51200000	00000000
544500	56999999	48786762	52469352	50277382	00000000
544500	55999999	50104857	52352163	50369686	00000000
544500	54999999	51140993	52261905	50497087	00000000
544500	53999999	52166864	52221298	50588299	00000000
544500	52999999	53193984	52190359	50683914	00000000
544500	51999999	54252211	52146412	50889201	00000000
544500	50999999	55395027	51934793	51139271	00000000
544500	49999999	56529538	51697340	51186695	00000000
544500	49100000	57562901	51656009	51198457	00000000
544500	48100000	58566833	51651459	51199843	00000000
544500	47100000	59567232	51651000	51199984	00000000
544500	46100000	60567272	51650954	51199998	00000000
544500	45100000	61567276	51650950	51199999	00000000
544500	44100000	62567276	51650949	51200000	00000000
544500	43100000	63567276	51650949	51200000	00000000
544200	56999999	48710652	52484978	50268445	00000000
544200	55999999	49930453	52370411	50351474	00000000
544200	54999999	51126046	52273431	50476133	00000000
544200	54965878	51130983	52272421	50477900	44420000
544200	54630957	51209333	52249273	50496285	49259927
544200	54398107	51344642	52242540	50517015	49197615
544200	54295477	51475449	52245329	50530673	00000000
544200	53999999	52150329	52229263	50567861	00000000
544000	56999999	48660529	52496933	50261987	00000000
544000	55999999	49854584	52384091	50338955	00000000
544000	55270450	50378674	52320505	50406202	44560000
544000	55251188	50422727	52295598	50406924	49335031
544000	55158489	50743658	52218785	50420745	50174312

Table 1--continued

Temperature, T ($^{\circ}$ K)	Pressure, P (atm)	Volume, v (cc/gm)	Molecular Weight, M	Moles of Gas, n	Moles of Solid, n _s
544000	54999999	51121863	52188671	50441266	50248768
544000	54630957	51197046	52173589	50462434	50287551
544000	54398107	51318258	52165928	50482168	50302447
544000	54251188	51514744	52162971	50500144	50298707
544000	54158489	51834148	52163656	50516892	50278615
544000	53999999	52135499	52167762	50533330	50242708
544000	53630957	52220793	52175747	50550521	50190256
544000	53398106	52361217	52188933	50569564	50119514
544000	53251188	52593881	52210160	50591561	49279185
544000	53222550	52677424	52217720	50597968	44600000
544000	52999999	53157002	52209065	50622724	00000000
544000	51999999	54184533	52177874	50731919	00000000
544000	50999999	55246105	52133373	50976131	00000000
544000	49999999	56371605	51883300	51147390	00000000
544000	48999999	57475841	51689807	51188733	00000000
544000	47999999	58501252	51654836	51198813	00000000
544000	46999999	59503947	51651335	51199881	00000000
544000	46100000	60504215	51650988	51199988	00000000
544000	45100000	61504242	51650953	51199998	00000000
544000	44100000	62504245	51650950	51199999	00000000
544000	43100000	63504245	51650949	51200000	00000000
543500	56999999	48531299	52540578	50240834	00000000
543500	55999999	49672032	52427373	50304627	00000000
543500	55599437	50119776	52400020	50325458	43700000
543500	55398107	50300173	52213589	50315045	50294487
543500	55251188	50483483	52166967	50334107	50445625
543500	55158489	50732824	52144892	50362126	50536399
543500	54999999	51111831	52131511	50391169	50598779
543500	53999999	52110239	52107783	50485747	50722142
543500	52999999	53115440	52106625	50521934	50699069
543500	51999999	54127990	52115388	50580067	50548211
543500	50999999	55163771	52155255	50742366	49961850
543500	50736530	55232754	52167536	50777085	44420000
543500	50100000	56219044	52131119	50992913	00000000
543500	49100000	57311210	51922877	51141069	00000000
543500	48100000	58403682	51711471	51182986	00000000
543500	47100000	59437504	51656471	51198317	00000000
543500	46100000	60440860	51651474	51199839	00000000
543500	45100000	61441179	51651001	51199984	00000000
543500	44100000	62441211	51650954	51199998	00000000
543500	43100000	63441214	51650950	51199999	00000000

Table 1--continued

Temperature, T ($^{\circ}$ K)	Pressure, P (atm)	Volume, v (cc/gm)	Molecular Weight, M	Moles of Gas, n	Moles of Solid, n _s
543000	56999999	48386366	52637164	50204327	00000000
543000	55999999	49475924	52517265	50251689	00000000
543000	55891642	49541423	52509945	50255301	44110000
543000	54999999	50998952	521117071	50358280	50753770
543000	53999999	51927247	51955178	50470232	50892759
543000	52999999	52949761	51915446	50500194	50921952
543000	51999999	53970888	51908332	50513239	50920045
543000	50999999	55102801	51901646	50543640	50900273
543000	49999999	56120084	51885011	50635058	50835994
543000	48999999	57160977	51862901	50851316	50657429
543000	48112256	58206480	52106208	51122579	44350000
543000	48100000	58235102	52104711	51124332	00000000
543000	47100000	59298521	51824661	51157870	00000000
543000	46100000	60364291	51675775	51192652	00000000
543000	45100000	61377141	51652750	51199448	00000000
543000	44100000	62378085	51651119	51199947	00000000
543000	43100000	63378174	51650966	51199994	00000000
542500	56999999	48274448	52747497	50174167	00000000
542500	56114815	49254792	52701266	50185649	00000000
542500	56114287	49256024	52701112	50185690	00000000
542500	56113762	49257263	52700959	50185731	00000000
542500	56113239	49258507	52700804	50185772	00000000
542500	56113133	49258761	52700773	50185780	43400000
542500	55999999	49562283	52524552	50184531	49636609
542500	55630957	50237908	52202327	50206617	50436845
542500	55398107	50367846	52147954	50242323	50637611
542500	55251188	50477446	52131435	50273860	50716667
542500	55158489	50625239	52122282	50301495	50763168
542500	54999999	50857718	52115515	50328077	50798958
542500	53999999	51747785	51941465	50449286	50933557
542500	52999999	52782258	51883293	50493777	50980138
542500	51999999	53790221	51875035	50501216	50986609
542500	50999999	54797711	51871790	50506209	50987153
542500	49999999	55819286	51864218	50519925	50986523
542500	48999999	56886598	51841654	50562645	50984188
542500	47999999	58108061	51783042	50685768	50976848
542500	46999999	59141352	51702586	50897035	50955974
542500	46100000	60163956	51692654	51104048	50839095
542500	45174800	61128698	51911913	51142765	44290000

Table 1--continued

Temperature, T ($^{\circ}$ K)	Pressure, P (atm)	Volume, v (cc/gm)	Molecular Weight, M	Moles of Gas, n	Moles of Solid, n _s
542500	45100000	61233264	51879471	51148032	00000000
542500	44100000	62289392	51708896	51183651	00000000
542500	43100000	63313736	51653891	51199100	00000000
542000	56999999	48210818	52778485	50167234	00000000
542000	56135357	49156437	52775064	50167972	44270000
542000	55999999	49354477	52642249	50169776	49329331
542000	55630957	50245382	52190983	50200030	50481652
542000	55398107	50375070	52138342	50239290	50701779
542000	55251188	50449589	52129158	50261323	50746666
542000	55158489	50550018	52124148	50278603	50770060
542000	54999999	50709485	52119957	50295660	50789644
542000	53999999	51546380	51998741	50402955	50900584
542000	52999999	52612004	51889818	50482162	50980945
542000	51999999	53628395	51870699	50498146	50997089
542000	50999999	54630601	51868452	50500199	50998903
542000	49999999	55631897	51867730	50501258	50999092
542000	49100000	56635408	51866109	50504046	50999111
542000	48100000	57646441	51861097	50512799	50999108
542000	47100000	58681182	51845693	50540357	50999090
542000	46100000	59786673	51802123	50624039	50999027
542000	45100000	61102704	51717882	50814716	50998810
542000	44100000	62121821	51662869	50966365	50997671
542000	43100000	63126373	51654383	51100247	50987031
541500	56999999	48157591	52781067	50166682	00000000
541500	56162290	48971113	52781014	50166693	43500000
541500	56158489	48996972	52780757	50166687	46611600
541500	55999999	49201300	52733200	50167495	49100685
541500	55398107	50369871	52133734	50239734	50733760
541500	54999999	50578744	52126077	50266582	50766033
541500	53999999	51340519	52113618	50323046	50822809
541500	52999999	52407108	51962423	50426414	50926316
541500	51999999	53462126	51881655	50488339	50988315
541500	51100000	54471606	51869376	50498765	50998744
541500	50100000	55472628	51868077	50499887	50999863
541500	49100000	56472759	51867929	50500030	50999976
541500	48100000	57472859	51867861	50500136	50999988
541500	47100000	58473143	51867686	50500437	50999989
541500	46100000	59474039	51867139	50501384	50999989
541500	45100000	60476870	51865412	50504379	50999989
541500	44100000	61485820	51860001	50513845	50999989
541500	43100000	62513987	51843403	50543636	50999990

Table 1--continued

Temperature, T (°K)	Pressure, P (atm)	Volume, v (cc/gm)	Molecular Weight, M	Moles of Gas, n	Moles of Solid, n _s
541000	56999999	48105051	52781139	50166666	00000000
541000	56176245	48596084	52781135	50166666	44810000
541000	55999999	49112377	52772525	50166831	48169335
541000	55398107	50355518	52131954	50243377	50743251
541000	54999999	50479275	52129739	50251738	50751733
541000	53999999	51197611	52127148	50261960	50761960
541000	52999999	52185720	52120700	50289309	50789310
541000	51999999	53229084	52106214	50362865	50862865
541000	51100000	54291261	51914218	50462030	50962028
541000	50100000	55312168	51873454	50495257	50995260
541000	49100000	56314847	51868496	50499512	50999513
541000	48100000	57315122	51867990	50499950	50999951
541000	47100000	58315150	51867939	50499994	50999995
541000	46100000	59315152	51867934	50499998	50999999
541000	45100000	60315153	51867933	50499999	50999999
541000	44100000	61315154	51867932	50500000	51100000
541000	43100000	62315156	51867930	50500004	51100000
535000	56999999	47525256	52781139	50166666	00000000
535000	56158562	48331261	52781140	50166666	43100000
535000	55999999	48525878	52781062	50166668	46144400
535000	55398107	50339057	52130497	50248821	50748821
535000	54999999	50398620	52130201	50249957	50749957
535000	53999999	51110796	52130174	50250060	50750061
535000	52999999	51820626	52130128	50250236	50750236
535000	51999999	52793485	52129992	50250761	50750761
535000	51100000	53795802	52129565	50252410	50752412
535000	50100000	54811962	52128233	50257630	50757627
535000	49100000	55863594	52124221	50274022	50774021
535000	48100000	57101790	52113606	50322987	50822989
535000	47100000	58133507	51966335	50423625	50923629
535000	46100000	59153662	51882550	50487580	50987576
535000	45100000	60157157	51869476	50498668	50998669
535000	44100000	61157534	51868088	50499865	50999865
535000	43100000	62157572	51867949	50499985	50999986

Table 2

SUMMARY OF COMPUTED VALUES OF DENSITY, SPECIFIC ENTHALPY,
SPECIFIC ENERGY, AND SPECIFIC ENTROPY FOR POLYSTYRENE
AT VARIOUS TEMPERATURES AND PRESSURES

Tempera- ture, T (°K)	Pressure, P (atm)	Density, d (gm/cc)	Enthalpy, h (cal/gm)	Energy, u (cal/gm)	Entropy, s (cal/ deg-gm)
546000	56999999	52828220	54617032	54587792	51287898
546000	55999999	51586775	54666869	54625597	51309590
546000	54999999	50451713	54732600	54678988	51338831
546000	53999999	49356936	54852175	54784327	51381790
546000	52999999	48227480	55126534	55115888	51492662
546000	51999999	47146870	55194961	55178472	51650083
546000	50999999	46134010	55213905	55195834	51748816
546000	49999999	45132396	55216535	55198243	51823116
546000	48999999	44132229	55216811	55198497	51893833
546000	47999999	43132212	55216839	55198522	51964170
546000	46999999	42132210	55216842	55198525	52103446
546000	45999999	41132210	55216842	55198525	52110476
546000	44999999	40132210	55216842	55198525	52117505
546000	44100000	39132210	55216842	55198525	52124535
546000	43100000	38132210	55216842	55198525	52131564
545500	56999999	52944430	54569451	54543809	51279618
545500	55999999	51677646	54613003	54577266	51300217
545500	54999999	50518367	54670603	54623885	51328048
545500	53999999	49427293	54751212	54694536	51364251
545500	52999999	48312445	54976390	54898881	51432532
545500	51999999	47184609	55164388	55151270	51596617
545500	50999999	46149741	55204678	55188505	51732686
545500	49999999	45144828	55211902	55195181	51815044
545500	48999999	44144290	55212720	55195937	51886712
545500	47999999	43144235	55212803	55196013	51957146
545500	46999999	42144230	55212812	55196021	52102745
545500	45999999	41144229	55212812	55196022	52109775
545500	44999999	40144229	55212812	55196022	52116804
545500	44100000	39144229	55212812	55196022	52123834
545500	43100000	38144229	55212813	55196022	52130863
545000	56999999	53108841	54521944	54499694	51270562
545000	55999999	51795897	54559125	54528697	51289946
545000	54999999	50600994	54611245	54570949	51316735
545000	53999999	49506402	54669228	54621406	51348645
545000	52999999	48408935	54792845	54733625	51397667
545000	51999999	47270260	55118073	55109113	51508303
545000	50999999	46178318	55183978	55170397	51692936

Table 2--continued

Temperature, T (°K)	Pressure, P (atm)	Density, d (gm/cc)	Enthalpy, h (cal/gm)	Energy, u (cal/gm)	Entropy, s (cal/ deg-gm)
545000	49999999	45161054	55205486	55190450	51802761
545000	48999999	44158879	55208452	55193212	51878569
545000	47999999	43158677	55208761	55193500	51949440
545000	47100000	42158655	55208792	55193528	52101979
545000	46100000	41158653	55208796	55193531	52109009
545000	45100000	40158652	55208796	55193532	52116038
545000	44100000	39158652	55208796	55193532	52123068
545000	43100000	38158652	55208796	55193532	52130097
544500	56999999	53127103	54474185	54455132	51260497
544500	55999999	51953678	54505215	54479821	51278586
544500	54999999	50709254	54552876	54518731	51304436
544500	53999999	49599289	54598700	54558290	51333800
544500	52999999	48515505	54664954	54622776	51371850
544500	51999999	47396492	54851280	54790201	51439252
544500	50999999	46253147	55136188	55126621	51591703
544500	49999999	45188843	55189704	55176880	51769164
544500	49100000	44177651	55203079	55189447	51867210
544500	48100000	43176418	55204624	55190897	51940724
544500	47100000	42176294	55204780	55191043	52101134
544500	46100000	41176232	55204795	55191058	52108167
544500	45100000	40176281	55204797	55191059	52115196
544500	44100000	39176280	55204797	55191059	52122226
544500	43100000	38176280	55204797	55191059	52129255
544200	56999999	53140715	54444898	54427688	51253760
544200	55999999	52107474	54472831	54450298	51271139
544200	54999999	50793358	54517734	54487209	51296355
544200	54965878	50763455	54518425	54487787	51296773
544200	54630957	50477706	54520116	54488130	51300353
544200	54398107	50290155	54530192	54496965	51306328
544200	54295477	50210327	54540639	54506617	51311201
544200	53999999	49665205	54559730	54523324	51324841
544000	56999999	53151393	54424619	54408623	51248812
544000	55999999	52117015	54451110	54430415	51265840
544000	55270450	51264079	54474338	54449536	51279062
544000	55251188	51236559	54467877	54442162	51277913
544000	55158489	51134470	54443118	54414575	51274880

Table 2--continued

Tempera- ture, T (°K)	Pressure, P (atm)	Density, d (gm/cc)	Enthalpy, h (cal/gm)	Energy, u (cal/gm)	Entropy, s (cal/ deg-gm)
544000	54999999	50820593	54433659	54404147	51275864
544000	54630957	50507493	54432229	54402120	51278940
544000	54398107	50314210	54435967	54405284	51283374
544000	54251188	50194271	54443766	54412454	51288892
544000	54158489	50119882	54455403	54423387	51295446
544000	53999999	49738007	54471175	54438361	51303119
544000	53630957	49452912	54491730	54457993	51312088
544000	53398106	49276841	54517990	54483165	51322598
544000	53251188	49168383	54551094	54514968	51334956
544000	53222550	49147617	54561092	54524581	51338554
544000	52999999	48636930	54578840	54540818	51350441
544000	51999999	47541907	54667253	54622564	51396117
544000	50999999	46406330	54886582	54826982	51480388
544000	49999999	45269102	55139950	55130951	51651005
544000	48999999	44210154	55187906	55176383	51830918
544000	47999999	43199500	55199496	55187357	51928586
544000	46999999	42198433	55200691	55188487	52100170
544000	46100000	41198327	55200810	55188599	52107228
544000	45100000	40198317	55200822	55188610	52114260
544000	44100000	39198316	55200823	55188611	52121290
544000	43100000	38198316	55200823	55188611	52128319
543500	56999999	53188217	54365676	54352810	51233018
543500	55999999	52148802	54393911	54377636	51250542
543500	55599437	51834887	54401717	54384329	51255231
543500	55398107	51333140	54344901	54315961	51241928
543500	55251188	51206832	54317607	54288196	51238015
543500	55158489	51136458	54304470	54276343	51238049
543500	54999999	50894199	54298313	54271231	51239917
543500	53999999	49907117	54300310	54273614	51257928
543500	52999999	48866244	54323257	54295301	51282424
543500	51999999	47781306	54397426	54366430	51322832
543500	50999999	46610605	54616352	54576691	51408167
543500	50736530	46429636	54663492	54621976	51425180
543500	50100000	45456529	54855224	54802177	51506625
543500	49100000	44321325	55127587	55120050	51668620
543500	48100000	43247719	55176876	55167100	51866704
543500	47100000	42228569	55194981	55184386	51986311
543500	46100000	41226829	55196698	55186027	52106128
543500	45100000	40226664	55196860	55186176	52113202
543500	44100000	39226648	55196876	55186191	52120235
543500	43100000	38226647	55196878	55186193	52127265

Table 2--continued

Temperature, T (°K)	Pressure, P (atm)	Density, d (gm/cc)	Enthalpy, h (cal/gm)	Energy, u (cal/gm)	Entropy, s (cal/ deg-gm)
543000	56999999	53258821	54278011	54268654	51205861
543000	55999999	52210117	54312990	54301465	51225413
543000	55891642	52184698	54315236	54303545	51226605
543000	54999999	51100104	54211489	54187297	51213251
543000	53999999	50107846	54215424	54192968	51231925
543000	52999999	49105289	54220297	54197297	51251018
543000	51999999	48102998	54229520	54206008	51271920
543000	50999999	46972744	54258426	54233530	51300035
543000	49999999	45832743	54347284	54318202	51350087
543000	48999999	44621205	54564196	54525211	51448135
543000	48112256	43484308	55102645	54970327	51635742
543000	48100000	43425346	55104374	54986811	51643683
543000	47100000	42334984	55141737	55134508	51817794
543000	46100000	41274505	55184329	55175507	52102191
543000	45100000	40265152	55192346	55183213	52111802
543000	44100000	39264490	55192909	55183753	52119011
543000	43100000	38264428	55192961	55183803	52126058
542500	56999999	53364367	54193105	54186459	51175121
542500	56114815	52392475	54203585	54196501	51185223
542500	56114287	52390587	54203619	54196533	51185249
542500	56113762	52388707	54203654	54196566	51185276
542500	56113239	52386835	54203688	54196599	51185303
542500	56113133	52386455	54203695	54196605	51185308
542500	55999999	52177846	54200690	54187073	51184622
542500	55630957	51420329	54194025	54157672	51186787
542500	55398107	51271852	54172768	54137304	51185132
542500	55251188	51209447	54158814	54129771	51185488
542500	55158489	51159938	54151871	54127873	51187566
542500	54999999	51116588	54149256	54128485	51190619
542500	53999999	50133728	54158177	54140068	51211131
542500	52999999	49127834	54164257	54145313	51230703
542500	51999999	48126546	54166157	54147020	51249017
542500	50999999	47125358	54169876	54150558	51268203
542500	49999999	46122057	54181452	54161612	51290822
542500	48999999	45112790	54217721	54196250	51324216
542500	47999999	43925401	54322429	54296259	51387697
542500	46999999	42707453	54504146	54469915	51488190
542500	46100000	41609918	54652951	54613245	51581862
542500	45174800	407777009	55118417	55112969	51825422

Table 2--continued

Temperature, T (°K)	Pressure, P (atm)	Density, d (gm/cc)	Enthalpy, h (cal/gm)	Energy, u (cal/gm)	Entropy, s (cal/ deg-gm)
542500	45100000	40428698	55124814	55119165	51863398
542500	44100000	39345551	55169155	55162147	52109853
542500	43100000	38318739	55188056	55180458	52124245
542000	56999999	53474340	54143209	54138103	51153028
542000	56135357	52639231	54143874	54138746	51158475
542000	55999999	52282105	54144941	54136356	51159974
542000	55630957	51407527	54141200	54103706	51163164
542000	55398107	51266616	54119708	53835479	51161397
542000	55251188	51222425	54107581	53802325	51162609
542000	55158489	51181812	54101473	53803632	51165082
542000	54999999	51140947	53988536	53816718	51168144
542000	53999999	50183022	54108238	53950067	51188841
542000	52999999	49163397	54120510	54105689	51211215
542000	51999999	48159135	54123117	54107899	51229882
542000	50999999	47158578	54123625	54108354	51247696
542000	49999999	46158253	54124382	54109079	51265672
542000	49100000	45157379	54126690	54111303	51284484
542000	48100000	44154692	54133982	54118327	51305971
542000	47100000	43146803	54156944	54140448	51335870
542000	46100000	42127117	54226673	54207622	51390940
542000	45100000	40973668	54385576	54360704	51495399
542000	44100000	39820873	54512231	54482729	51590493
542000	43100000	38791306	54545340	54514735	51641787
541500	56999999	53634551	54104349	54100533	51130731
541500	56162290	53102974	54104360	54100544	51135366
541500	56158489	53100303	54104356	54100530	51135423
541500	55999999	52496768	54104742	53998672	51136917
541500	55398107	51270363	53757015	53400419	51136023
541500	54999999	51172787	53545915	53405759	51142711
541500	53999999	50293668	53566060	53483596	51159128
541500	52999999	49245634	53732771	53634181	51183869
541500	51999999	48216391	53836812	53724898	51207181
541500	51100000	47212041	53854394	53740184	51225768
541500	50100000	46211582	53856356	53741898	51243456
541500	49100000	45211523	53856792	53742303	51261058
541500	48100000	44211479	53857593	53743079	51278688
541500	47100000	43211352	53860068	53745485	51296435
541500	46100000	42210952	53867888	53753088	51314559
541500	45100000	41209700	53892614	53777129	51333873
541500	44100000	40205837	53970768	53853116	51356945
541500	43100000	39194557	54121671	54109223	51391828

Table 2--continued

Temperature, T ($^{\circ}$ K)	Pressure, P (atm)	Density, d (gm/cc)	Enthalpy, h (cal/gm)	Energy, u (cal/gm)	Entropy, s (cal/ deg-gm)
541000	56999999	53951916	53694001	53668561	51102507
541000	56176245	53167761	53694003	53668561	51106923
541000	55999999	52889860	53694489	53667274	51108423
541000	55398107	51281279	53398548	52557914	51106906
541000	54999999	51208648	53173222	52571549	51112645
541000	53999999	50506042	53119444	52715885	51123287
541000	52999999	49538443	53157181	53112205	51137378
541000	51999999	48436519	53277706	53222228	51160787
541000	51100000	47343333	53441226	53370690	51191754
541000	50100000	46320339	53496049	53420451	51214230
541000	49100000	45317614	53503066	53426819	51232439
541000	48100000	44317336	53503788	53427474	51250079
541000	47100000	43317309	53503861	53427540	51267659
541000	46100000	42317306	53503869	53427548	51285233
541000	45100000	41317305	53503873	53427551	51302807
541000	44100000	40317304	53503883	53427561	51320382
541000	43100000	39317302	53503914	53427592	51337959
535000	56999999	54190383	53420163	53407442	50654783
535000	56158562	53301875	53420163	53407442	50701635
535000	55999999	53190158	53420166	53407431	50713369
535000	55398107	51294934	53129751	-53197136	50701116
535000	54999999	51250865	-52993682	-53195903	50757167
535000	53999999	50902556	-53168349	-53195181	50846512
535000	52999999	50121858	-53175009	-53194882	50935051
535000	51999999	49126026	-53174925	-53194141	51102464
535000	51100000	48125659	-53172546	-53191818	51111790
535000	50100000	47123158	-53164816	-53184480	51122284
535000	49100000	46115795	-53140495	-53161409	51136438
535000	48100000	44982409	-52678428	-52924937	51161314
535000	47100000	43749023	52814730	52491412	51204207
535000	46100000	42650776	53176350	53139137	51239437
535000	45100000	41636305	53192807	53154748	51260125
535000	44100000	40634782	53194583	53156432	51278035
535000	43100000	39634629	53194762	53156602	51295643

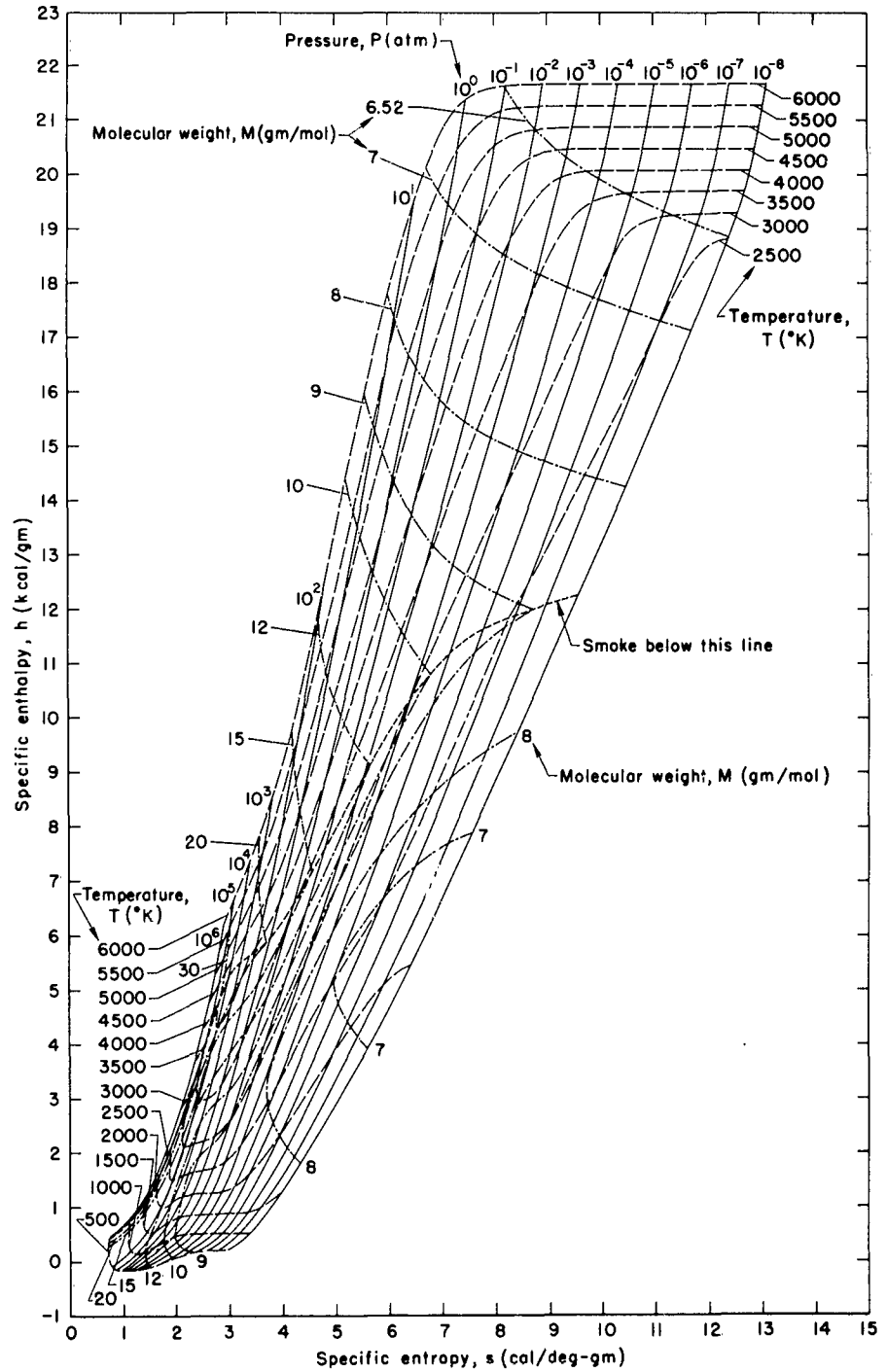


Fig. 1—Specific enthalpy versus specific entropy for polystyrene with cross plots of temperature, pressure, and molecular weight

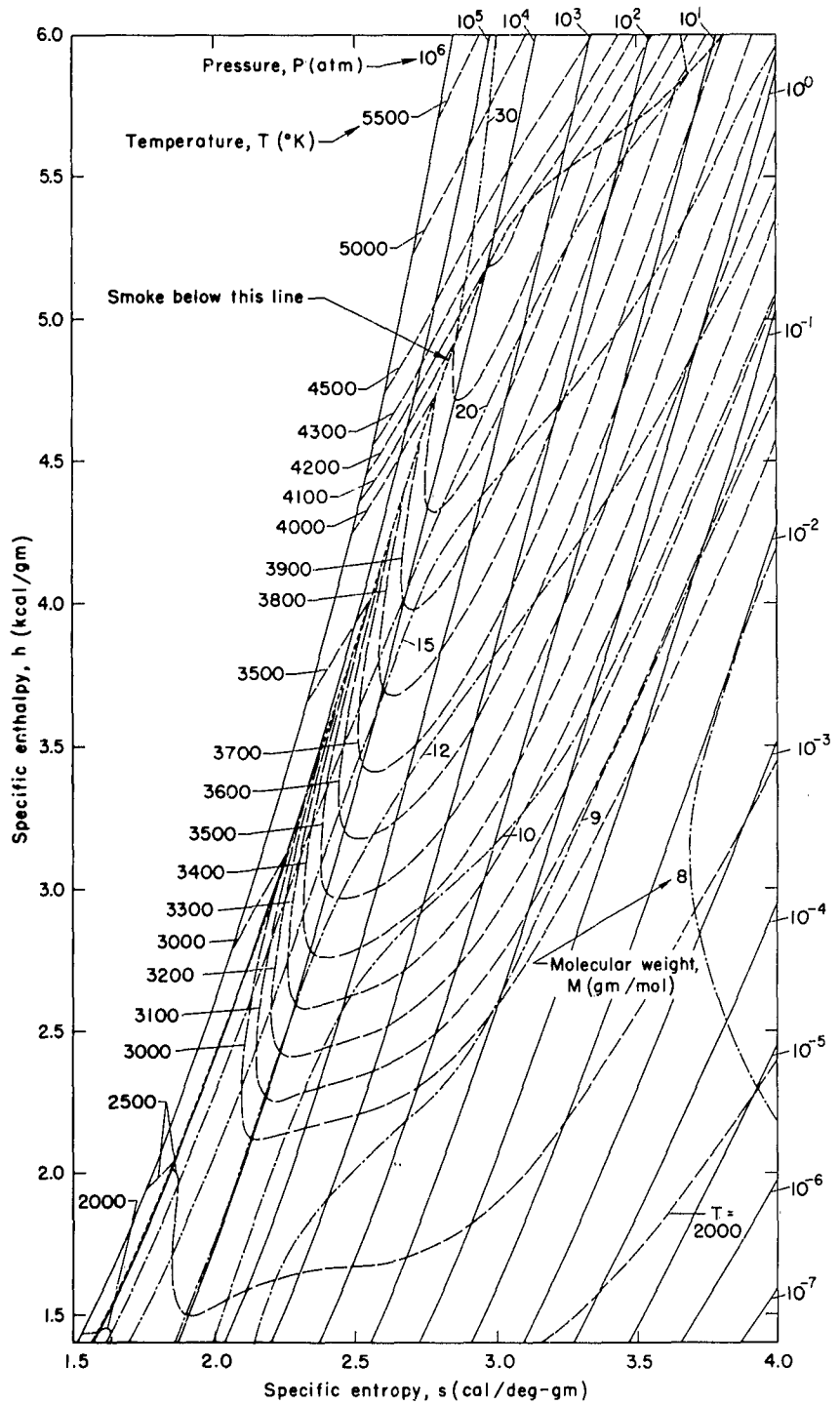


Fig. 1a — Detail of Fig. 1

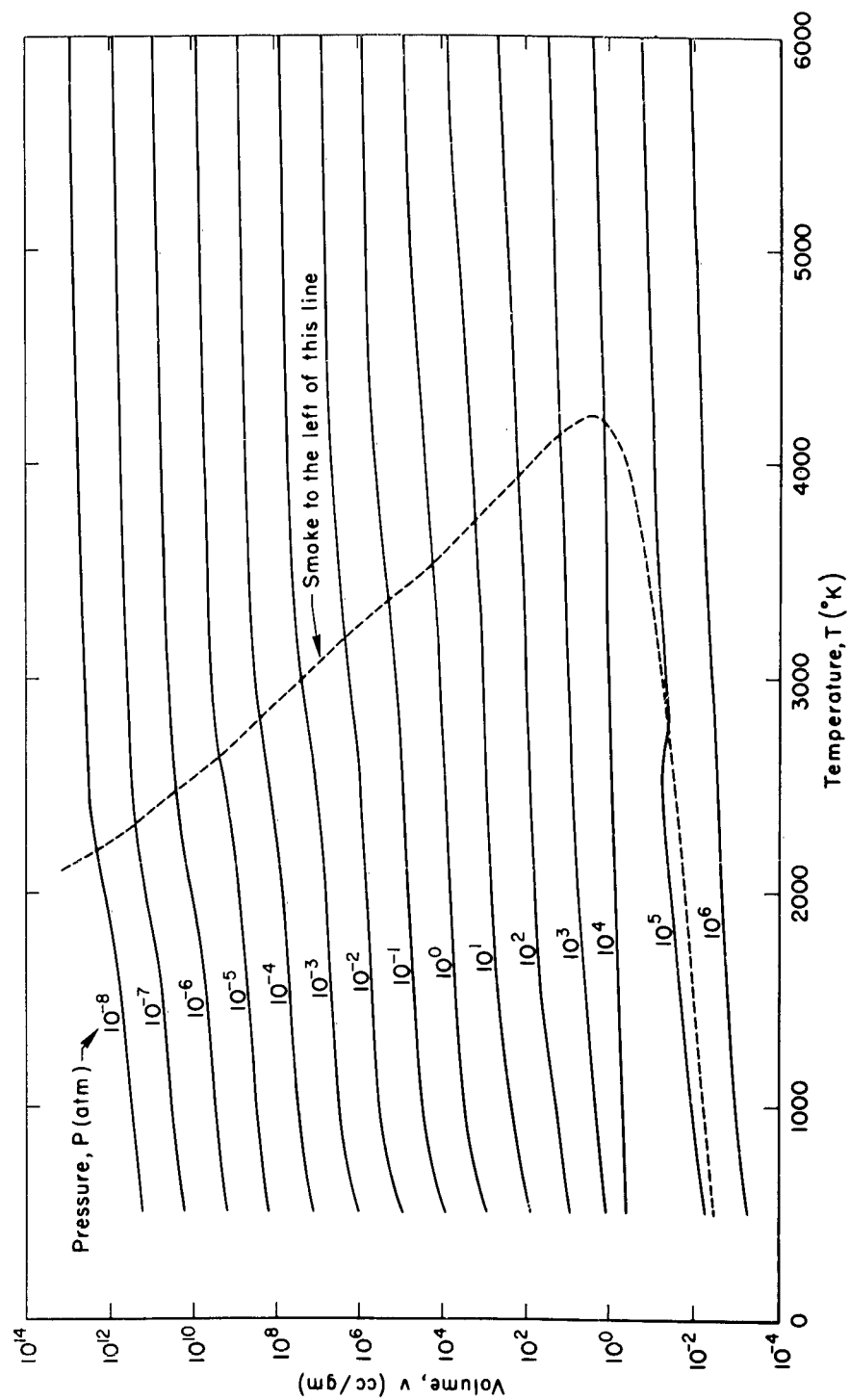


Fig. 2—Volume versus temperature for polystyrene with cross plots of constant pressure